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ANFIS modelling for theoretical evaluation of ultrasonic velocities in binary liquid mixtures

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Abstract : "Adaptive Neuro Fuzzy Inference System" – the ANFIS, a newly developed technique is applied for the first time to compute the velocity of ultrasonic waves in binary liquid mixtures. To test the validity of this method, three binary liquid systems, each with different nature of molecular interaction are studied. The computed values of U_{mix} are reported and compared with those obtained using some other theories.

Keywords : ANFIS, binary liquid mixtures, ultrasonic velocity.

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1. Introduction

Ultrasonic velocities in binary liquid mixtures can be calculated theoretically using Jacobson's Free Length Theory (FLT) [1], Schaaff's Collision Factor Theory (CFT) [2], Nomoto's empirical relation (NOM) [3], *etc.* The accuracy in the predicted values of U_{mix} from these theories and relations, differ according to the type of liquids involved in the binary system. Nomoto's relation and CFT are very much suitable for polar liquids and FLT for non-polar liquids. Hence, an attempt has been made to compute the ultrasonic velocity in pure liquids and liquid mixtures of any type through the Adaptive Neuro Fuzzy Inference System.

Boolean logic is a *two-level* logic in which an element (parameter) is viewed as entirely TRUE or FALSE. It is useful for analysing *simple* and *linear* problems, since a small change in input can cause abrupt change in output. Fuzzy logic is a *multi-level* logic. It is useful for analysing complex and nonlinear problems because small changes in input, result in a more graceful change in the output. Fuzzy logic is a convenient way of mapping an input into an output space.

In Fuzzy logic, a parameter is represented by a membership value, which lies between 0 and 1. The membership function of inputs and outputs are connected by simple IF-THEN rules, which are written based on experts' (previous) knowledge. The Fuzzy Inference System (FIS) learns from these rules and then becomes capable of predicting the relationship between any new set of input-output parameters.

A Neural Network (NN) is a technique to implement intelligence, using models that simulate the working network of the neurons in the human brain [4–6]. A neuron refers to the processing element in the Artificial Neural Network (ANN). The most important feature of NNs is their ability to achieve an accurate nonlinear mapping from input-output pairs of data without knowing their functional relationship [7].

Adaptive Neuro-Fuzzy Inference System, the ANFIS is the result of the integration of Fuzzy logic theory and Neural Networks. This hybridization makes ANFIS to inherently possess the advantages of both systems. The architecture and learning procedure underlying ANFIS is a Fuzzy Inference System implemented in the framework of NNs.

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The velocity of ultrasonic waves (u) in a liquid depends on many of the characteristic parameters of a liquid like molecular weight (M), density (ρ), viscosity (η), surface tension (σ), space filling factor (r_f), *etc.* Several approximate theories and empirical relations exist to connect the ultrasonic velocity with these parameters. For example, ultrasonic velocity is connected to surface tension through Aurbach Realtion [8], with molecular weight and density through Rao's rule and Nomoto's relation [3], with space filling factor through Schaaff's collision theory [2] and so on.

2. Methodology

The exclusive feature of ANFIS is that it *self-learns* and recognizes the exact input-output relationship from the Fuzzy Inference rules and so acquires enough intelligence in predicting a new situation. The learning process of ANFIS consists of training the FIS to understand the exact input-output relations using a set of data called 'Training Data' (TrnData) comprising of input-output parameters of a system under study. Then, the validity of the FIS can be tested by using another set of data known as 'Check Data' (ChkData), which comprises of identical input-output parameters but having different values. ANFIS generates automatically the Fuzzy rules and selects the rules with maximum firing strength. Now, the FIS is capable of predicting the output of a new environment of inputs. If a third data set called 'test data' comprising of input parameters alone is given, the ANFIS will predict the output parameters (For further details, reference can be made to 'Fuzzy logic Toolbox [9]).

In the present work, molecular weight (M), density (ρ), viscosity (η), surface tension (σ) and space filling factor (r_f) of pure liquids are taken as the input parameters and the corresponding ultrasonic velocities are taken as the output parameters. A training data set is constructed using the values of these parameters for forty pure liquids. A part of the training data set is shown in Table 1. A check data is constructed using the values of identical input-output parameters of another ten liquids. In the test data set, molecular weight (M), density (ρ), viscosity (η), surface-tension (σ) and space-filling factor (r_f) of a binary liquid system being studied, under varying concentrations are taken as input parameters. Now, the trained ANFIS predicts the ultrasonic velocities (outputs) in this binary system, which are our desired values.

Table 1. Characteristic parameters of pure liquids used as training data (TrnData).

Liquid	M ($\times 10^{-3}$ kg)	ρ (kg/m^3)	η ($\times 10^{-3}$ pascal sec)	σ ($\times 10^3$ N/m)	r_f	u (m/sec)
Methanol	32.04	786.8	0.544	22.07	0.914	1103
Acetonitrile	41.05	766.5	0.335	27.424	0.922	1245.1
Cyclohexane	84.16	773.9	0.894	24.65	0.2545	1318
Dimethyl acetamide	87.12	927.6	1.6852	31.277	0.9265	1420.2
Ethyl acetate	88.11	900.3	0.423	23.39	0.629	1116
Triethylamine	101.19	714.39	0.317	19.23	0.3209	1070
Ethyl benzene	106.17	853.88	0.571	27.654	0.325	1278
p-Xylene	106.17	847.97	0.545	26.93	0.2979	1269
n-Octane	114.23	698.6	0.508	21.14	0.2401	1192
Carbontetrachloride	153.82	1588	0.908	26.43	0.2921	926

The Block diagram of Sugeno type fuzzy inference system (one output only) used for the present work and the corresponding structure of ANFIS are shown in Figures 1, 2 respectively.

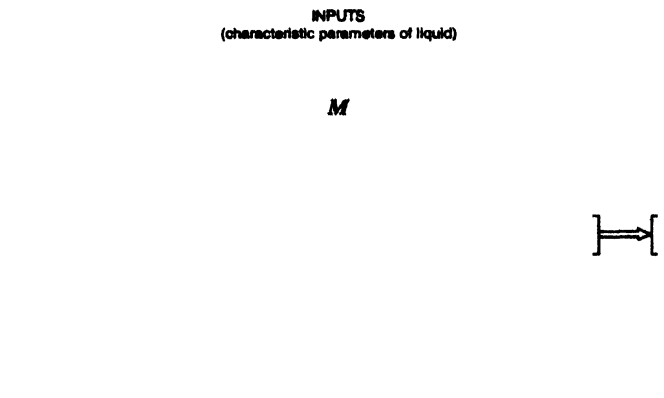
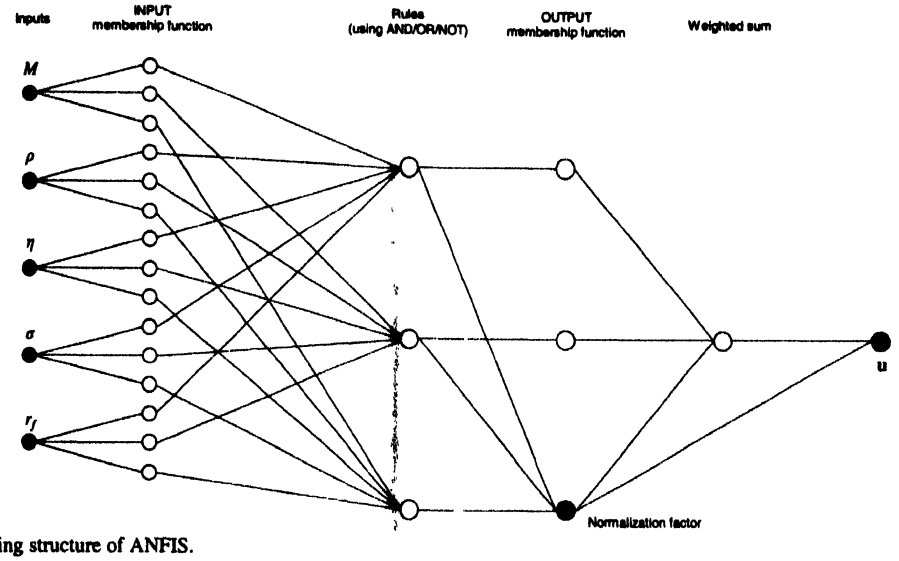


Figure 1. Sugeno-type fuzzy system for present work.



u (m/sec)

Figure 2. Corresponding structure of ANFIS.

The closeness of the predicted values of U_{mix} to the experimentally observed values, is tested by calculating the Average Percentage Error (APE) using the relation,

$$APE = \frac{1}{n} \cdot \sum \frac{U_{mix\,(obs)} - U_{mix\,(cal)}}{U_{mix\,(obs)}} \times 100\,\%$$

where

n → number of data used,

$U_{mix\,(obs)}$ → experimental values of ultrasonic velocities,

$U_{mix\,(cal)}$ → computed values of ultrasonic velocities.

To illustrate the applicability of this ANFIS technique, three binary liquid systems, each having different nature of intermolecular interaction are taken in the present study. The check data used, the computed values of U_{mix} and the APE values are presented in Tables 2–4.

Finally, the observed and computed U_{mix} values *versus* the mole fraction of first component are graphically given in Figures 3–5.

3. Results and discussion

In the case of Triethylamine (TEA) (μ = 0.66D) + Ethyl benzene (μ = 0.13D) [11] system, since both molecules are weakly polar and belong to same proton acceptor group, only weak dipole-dipole type of interaction can be expected. Therefore, the velocity *versus* mole fraction curve for this system will be slightly nonlinear and is shown in Figure 3.

In the case of TEA + p-xylene system, TEA is weakly polar and it has only H-acceptor sites and p-xylene is almost nonpolar with π electron configuration. So, only very weak intermolecular interaction of the type

Table 2. Characteristic parameters of binary mixtures used as check data, observed and predicted values of U_{mix} in triethylamine + ethyl benzene system.

Mole fraction of triethylamine	M_{mix} (×10⁻³ kg)	ρ_{mix} (kg/m³)	η_{mix} (×10⁻³ pascal sec)	σ_{mix} (×10³ N/m)	r_{fmix}	u^*_{exp} (m/sec)	Present work U_{ANFIS} (m/sec)	U_{NOM} (m/sec)	U_{CFT} (m/sec)	U_{FLT} (m/sec)
0	106.17	853.88	0.571	27.654	0.325	1278	1278	—	1278	1278
0.1366	105.49	834.83	0.536	26.503	0.3244	1248	1244	1245	1248	1238
0.2214	105.07	822.99	0.515	25.789	0.3240	1225	1225	1225	1230	1217
0.2775	104.79	815.17	0.5	25.316	0.3238	1212	1214	1212	1216	1202
0.4664	103.85	788.82	0.452	23.725	0.323	1172	1175	1171	1178	1162
0.5313	103.52	779.76	0.436	23.178	0.3228	1159	1161	1158	1164	1148
0.6297	103.03	766.04	0.411	22.349	0.3224	1140	1146	1138	1144	1129
0.7515	102.43	749.05	0.38	21.323	0.3219	1119	1121	1115	1119	1107
0.8390	101.99	736.85	0.357	20.586	0.3215	1103	1103	1098	1102	1095
0.9010	101.68	728.19	0.342	20.063	0.3213	1093	1090	1087	1089	1085
1.0000	101.19	714.39	0.317	19.23	0.3209	1070	1070	—	1070	1070
						APE =	0.234%	0.214%	0.224%	0.685%

* Velocity data taken from Ref. [10].

Table 3. Characteristic parameters of binary mixtures used as check data, observed and predicted values of U_{mix} in triethylamine + p-xylene system.

Mole fraction of triethylamine	M_{mix} ($\times 10^{-3}$ kg)	ρ_{mix} (kg/m^3)	η_{mix} ($\times 10^{-3}$ pascal sec)	σ_{mix} ($\times 10^3$N/m)	r_{fmix}	u^*_{exp} (m/sec)	Present work U_{ANFIS} (m/sec)	U_{NOM} (m/sec)	U_{CFT} (m/sec)	U_{FLT} (m/sec)
0	106.17	847.97	0.545	26.93	0.2979	1269	1269	—	1269	1269
0.1479	105.43	828.21	0.511	25.79	0.3013	1241	1240	1235	1238	1228
0.2592	104.88	813.35	0.486	24.93	0.3039	1221	1218	1210	1215	1202
0.3743	104.31	797.97	0.459	24.05	0.3065	1196	1195	1186	1192	1175
0.4750	103.8	784.52	0.437	23.27	0.3088	1177	1175	1166	1172	1155
0.5422	103.47	775.54	0.421	22.76	0.3103	1162	1160	1152	1158	1143
0.6925	102.72	755.46	0.387	21.59	0.3138	1132	1131	1124	1129	1116
0.7310	102.53	750.32	0.378	21.3	0.3147	1124	1123	1117	1121	1110
0.8309	102.03	736.98	0.355	20.53	0.3170	1105	1103	1099	1102	1086
0.8849	101.76	729.77	0.343	20.12	0.3183	1095	1093	1089	1092	1080
1.0000	101.19	714.39	0.317	19.23	0.3209	1070	1070	—	1070	1070
* Velocity data taken from Ref. [10].						APE =	0.117%	0.714%	0.264%	1.23%

Table 4. Characteristic parameters of binary mixtures used as check data, observed and predicted values of U_{mix} in acetonitrile + dimethyl acetamide system

Mole fraction of acetonitrile	M_{mix} ($\times 10^{-3}$ kg)	ρ_{mix} (kg/m^3)	η_{mix} ($\times 10^{-3}$ pascal sec)	σ_{mix} ($\times 10^3$N/m)	r_{fmix}	u^*_{exp} (m/sec)	Present work U_{ANFIS} (m/sec)	U_{NOM} (m/sec)	U_{CFT} (m/sec)	U_{FLT} (m/sec)
0	87.12	927.6	1.6852	31.277	0.9265	1420.2	1420.2	—	1420.2	1420.2
0.1631	79.61	901.3	1.4649	30.649	0.9258	1400.1	1397.3	1402	1407.5	1395.2
0.3048	73.08	878.5	1.2736	30.103	0.9251	1380.3	1375.5	1383.9	1388.5	1372.6
0.4291	67.35	858.5	1.1058	29.624	0.9246	1360.3	1356	1366.1	1367.9	1352.1
0.5390	62.29	840.8	0.9574	29.2	0.9241	1341.7	1338.4	1348.3	1346.9	1333.4
0.6369	57.78	824.9	0.8252	28.823	0.9236	1323.5	1322.1	1330.7	1328.3	1316.4
0.7246	53.74	810.9	0.7068	28.485	0.9232	1305.4	1306.8	1313.3	1308.3	1300.4
0.8036	50.09	798.1	0.6002	28.181	0.9229	1289.1	1291.7	1296	1290.6	1285.3
0.8752	46.79	786.6	0.5035	27.905	0.9226	1273.2	1276.5	1278.9	1273.3	1271.3
0.9404	43.79	776.1	0.4155	27.654	0.9223	1258.2	1260.7	1261.9	1259.9	1258
1.0000	41.05	766.5	0.335	27.424	0.922	1245.1	1245.1	—	1245.1	1245.1
* Velocity data taken from Ref. [10].						APE =	0.179%	0.409%	0.247%	0.325%

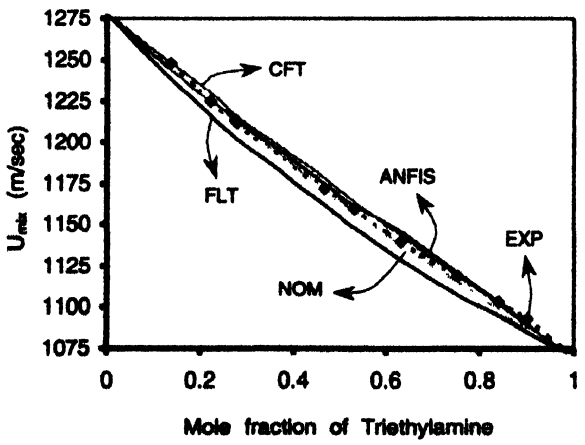


Figure 3. U_{mix} values *versus* mole fraction of triethylamine binary liquid mixture : triethylamine + ethyl benzene.

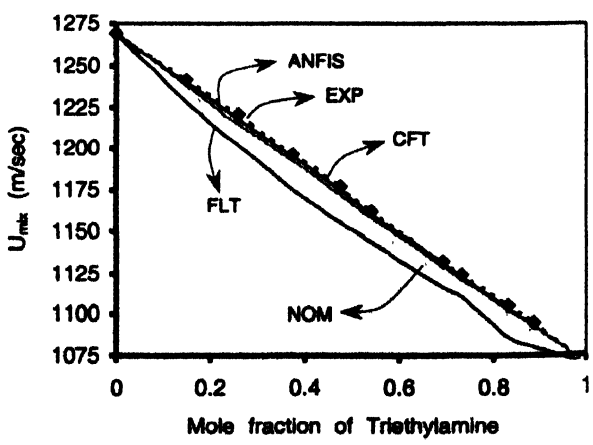


Figure 4. U_{mix} values *versus* mole fraction of triethylamine binary liquid mixture : triethylamine + pxylene.

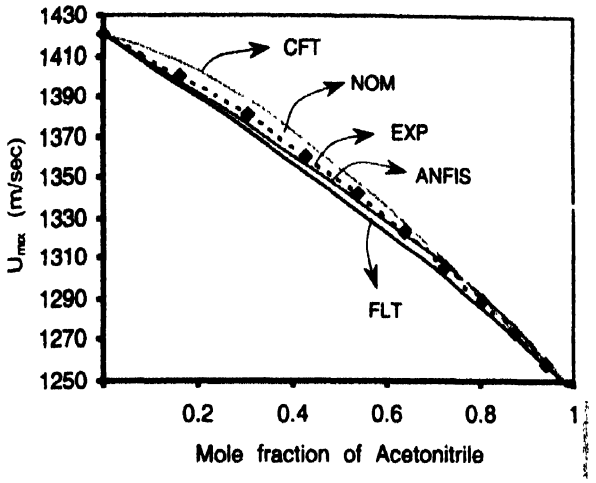


Figure 5. U_{mix} values *versus* mole fraction of acetonitrile binary liquid mixture : acetonitrile + dimethyl acetamide.

dipole-dipole interaction can be expected in this mixture. This fact is well exhibited in the U_{mix} values presented in Table 3 and in Figure 4.

Acetonitrile (ACN) is strongly polar (μ = 3.925D) and dimethyl acetamide (DMA) is also strongly polar (μ = 3.7D) [12]. So, in this binary system ACN + DMA, strong intermolecular interactions between unlike molecules can be expected and resulting variation of ultrasonic velocity with the mole fraction of ACN must be most nonlinear. This can be observed from the U_{mix} values presented in Table 4 and in Figure 5.

4. Conclusion

The ANFIS technique, which has a FIS structure similar to that of a neural network, can be successfully employed in the theoretical computation of ultrasonic velocities in binary liquid systems with significantly high accuracy compared to some of the other available theories.

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